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Properties of Ni-Al under shock loading

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Introduction

New models for the dynamic response of materials will be based increasingly on better understanding and representation of processes occurring at the microstructural level. These developments require advances in diagnostics and models which can be applied explicitly to microstructural response. Various phenomena occur at the microstructural level which are generally ignored or averaged out in continuum-level models. One example of such 'irregular hydrodynamics' is the roughness imparted to a shock wave as it propagates through a polycrystalline material.

We have developed imaging techniques to study spatial variations in shock propagation through polycrystalline materials. In order to interpret spatially-resolved data from polycrystal samples, we need to compare with simulations which represent the microstructure. Here we describe work undertaken to develop a model of the dynamic response of individual grains. The material chosen was Ni-Al alloy, because it exhibits a relatively large degree of elastic anisotropy, and it is relatively easy to manufacture.

Sample preparation

Pure powder Ni and Al were mixed in proportions to give equal numbers by atom and fused. A single crystal was grown by starting with a seed crystal at the surface of the melt and drawing it away. The resulting crystal was in the form of a bar of about 5 mm diameter. The orientation was determined by Laue diffraction, and the bar was sliced to obtain samples oriented parallel to (100) and (110) planes. Samples were cut to shapes suitable for the flyer experiments. They were then polished to the desired thicknesses, using grinding paste of successively smaller particles to obtain a mirror finish.

Theoretical equation of state and elasticity

An *ab initio* equation of state (EOS) was calculated using quantum mechanics, by the method applied previously to several elements [Swift00,Swift01]. The frozen-ion cold curve was estimated for Ni-Al in the CsCl structure by finding the ground state energy of the outer electrons with respect to *ab initio* pseudopotentials for Ni and Al. *Ab initio* phonons were deduced by performing additional calculations of a supercell with atoms displaced from equilibrium. A rigorous thermodynamically complete EOS was then generated in tabular form.

Because of the intrinsic limitations of the local density approximation used to represent the exchange-correlation energy of the outer electrons, the *ab initio* EOS overpredicted the lattice spacing at

STP by ~1%. This discrepancy was corrected by adding a constant pressure offset to the EOS.

The elastic response was predicted as a function of compression by performing further quantum mechanical calculations with the lattice cell compressed uniaxially or sheared.

Laser-launched flyer experiments

The theoretical EOS was tested, and a basic constitutive model obtained, by performing laser-launched flyer experiments with laser Doppler velocimetry (VISAR) diagnostics. Flyers were punched from copper foil and glued to a substrate consisting of PMMA coated with thin (~micron) layers of materials to absorb the laser energy, confine the plasma, and insulate the flyer from heating. The flyers were between 50 and 250 microns thick.

The TRIDENT laser at Los Alamos was used to launch the flyers. Pulses ~600 ns long in the infra-red were used, allowing the flyers to be launched without shocking up, spalling or significant ringing. Flyer speeds up to ~600 m/s were obtained.

The flyers were impacted against Ni-Al targets, attached to PMMA windows. The target typically covered half of the area of the flyer, giving space for the flyer speed to be measured with the VISAR. The surface of the target was also monitored with the VISAR. Wave profiles at the surface of the target provided EOS and strength information.

The Hugoniot data obtained were consistent with the *ab initio* EOS. The magnitude of the elastic precursor allowed an estimate to be made of the flow stress at different orientations.

Single-crystal plasticity model

The EOS, elasticity, and flow data were used to calibrate a continuum-type model for the response of a crystal of Ni-Al. The local state includes an orientation; plastic flow was based on the mechanical threshold stress (MTS) model [Johnson92,Goto00]. This model will be used for explicit microstructure simulations, complementing future experiments on bicrystals of Ni-Al.

Conclusions

The *ab initio* quantum mechanical method produced a complete EOS and elasticity model for Ni-Al alloy in the CsCl structure. The EOS was tested against laser-launched flyer experiments, which also allowed an orientation-dependent plastic flow model to be calibrated.

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